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Kants Hand, Chiralität und konvexe Polytope

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Abstract: Worin unterscheidet sich eine rechte von einer linken Hand, trifft doch jede Eigenschaft der einen Hand auch auf die andere zu? Diese von Kant gestellte Frage und die von ihm gegebene Antwort waren immer wieder Anlass zu Kontroversen über die Natur des Raumes. Einen klärenden Beitrag lieferte der Mathematiker Reidemeister, dessen Aussagen in dieser Arbeit unter Verwendung eines in der Chemie wichtigen Begriffs interpretiert werden, nämlich der Chiralität. Im Weiteren geht es um die Tragweite des aus dieser Deutung hervorgehenden Phänomens der Diachiralität und um das Bilden von Chiralitätsklassen chiraler Objekte durch Orientierung. In einem zweiten Teil werden die besprochenen Chiralitätsaspekte auf konvexe Polytope angewendet, wobei u.a. ein Minimierungsverfahren und ein darauf basierender Algorithmus wesentlich sind.

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Kant's hand, chirality and convex polytopes*

Karl Wirth and André S. Dreiding

Study of Hands by Leonardo da Vinci

manche meinen lechts und rinks kann man nicht velwechsern, werch ein illtum!	some imagine light and reft cannot be confused at arr, what an ellol!
Ernst Jandl	translated by *Eva Virag Jansen*

What is the difference between a right and a left hand albeit each property of one hand is always a property of the other? This question posed by Kant as well as his answer have been the source of controversies concerning the nature of space. A clarifying contribution was presented by the mathematician Reidemeister and his statements are interpreted in this work using an important concept from chemistry, namely chirality. As a consequence of this interpretation, the phenomenon of diachirality, which is of practical relevance, is examined. Furthermore, classifications of chiral objects by means of orientation are considered. In a second part, the discussed chiral aspects are applied to convex polytopes, whereby a minimizing procedure and a corresponding algorithm are essential.

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1 Kant's paradox

Immanuel Kant (1724-1804) is regarded as the great philosopher who concerned himself with the possibilities and limitations of human reason. Much was written of his philosophical works in 2004, the 200th anniversary of his death. Little is known, however, of his more mathematical and scientific writings, which result from his early period. In the essay *Concerning the ultimate ground of the differentiation of directions in space* [6], published in 1768, he dealt with a phenomenon which plays an outstanding role in modern science and which nowadays is denoted by the concept of chirality (Greek: cheir = hand). Kant states:

> *"The right hand is similar and equal to the left hand. And if one looks at one of them on its own, examining the proportion and the position of its parts to each other, and scrutinizing the magnitude of the whole, then a complete description of the one must apply in all respects to the other as well. (...)*
>
> *However, there is no difference in the relation of the parts of the hand to each other, and that is so whether it be a right hand or a left hand; it would therefore follow that the hand would be completely indeterminate in respect of such a property. In other words, the hand would fit equally well on either side of the human body; but that is impossible."*

Kant ascertained that two objects which are perceived to be different, such as a right and a left hand, could (ideally realized) coincide perfectly regarding their metrical properties: Each measured distance on one hand has a corresponding distance on the other; nowadays one says that the hands are isometric. Kant then formulated a paradox: Since both hands are isometric, they should each be able to fit either half of the body, which can (ideally realized) also be considered to be isometric. This contradicts our experience that each hand fits only one half of the body. How did Kant try to explain this contradiction?

> *"Our considerations make it plain that the determinations of space are not consequences of the positions of the parts of matter relative to each other. On the contrary, the latter are consequences of the former. Our considerations, therefore, make it clear that differences, and true differences at that, can be found in the constitution of bodies; these differences relate exclusively to absolute and original space, for it is only in virtue of absolute and original space that the relation of physical things to each other is possible. Finally, our considerations make the following point clear: absolute space is not an object of outer sensation; it is rather a fundamental concept which first of all makes possible all such outer sensation. For this reason, there is only one way in which we can perceive that which, in the form of a body, exclusively involves reference to pure space, and that is by holding one body against other bodies."*

Our interpretation of this rather arduous text is that the difference between isometric objects, such as our two hands, cannot be found in the objects themselves. It must lie somewhere else. Kant attributed the difference to a spacial property not explainable by mutual positions of the parts, i.e., by distances. He referred to a space with this property as being 'absolute'; in this regard, a right and a left hand are different. Here Kant sided with Newton, who, in a dispute with Leibniz, half a century earlier, had also postulated the idea of an absolute space with points eternally fixed. According to Leibniz, points need references to each other in order to be determined.

Leibniz' position gradually gained in acceptance and until the 20th century, and the more religiously influenced conceptions of an absolute space gave way to a logical-mathematical argumentation. In the course of time, several mathematicians have dealt with Kant's problem in various ways. It was, however, mainly K. Reidemeister who concerned himself thoroughly with Kant's paradox and provided arguments against his conclusions. He presented them in his book *Raum und Zeit* published in 1957 [9]. Reidemeister taught in 'Kant's' Königsberg from 1925 till 1933, was called to Marburg in 1934 and from 1955 he worked in Göttingen. His research was mainly in the field of geometry, in particular the fundamentals, as well as in combinatoric topology and knot theory. Before we concern ourselves with Reidemeister's thoughts, we shall explain the underlying phenomenon, namely that of chirality.

2 Chirality

The term chirality originated in the natural sciences, in particular in chemistry. It is not at all prevalent in mathematics and does not receive any mention in Reidemeister's book, although the concept permits a succinct interpretation of his result. The fact that chirality has received little attention in mathematics is all the more astonishing in that it is a purely geometric concept. Indeed, many appealing problems with a broad potential for applications are connected to chirality. With this article, we would like to help close an interdisciplinary gap. The following outline of the concept of chirality may be understood intuitively.

The word chirality was introduced in 1893 by the British physicist Lord Kelvin, but has only been commonly used since about 1960. Kelvin's definition was as follows: *"I call any geometrical figure, or group of points, chiral, and say that it has chirality, if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself* (. . .)*."* By the phrase 'brought to coincide with itself', Kelvin meant 'brought to coincide with itself by a proper movement', i.e., by rotation, translation or combinations thereof (realizable by a screw motion).

The simplest (spacial) figures which can be chiral consist of four non-coplanar points; they determine a tetrahedron (Fig. 1). The reader will easisly verify that, according to Kelvin's definition, tetrahedron T_1 with mutual different edge lengths a, b and c is chiral. Tetrahedron T_2 is not chiral, however; it is said to be *achiral.*

In the plane, chirality is analogously definable by using a reflection about a straight line. And clearly, by means of a reflection about a $(d{-}1)$ - dimensional hyperplane,

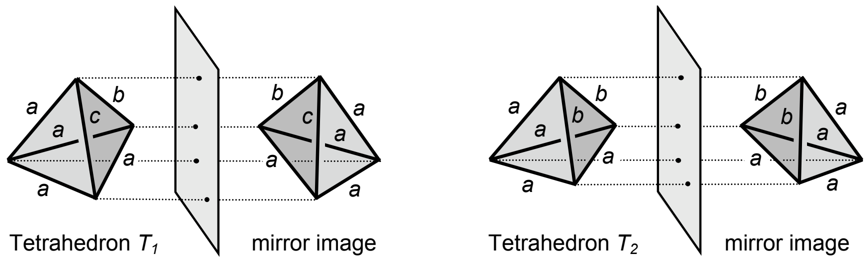


Fig. 1 Chiral and achiral figure and their mirror images in space

the concept can be extended to any d-dimensional Euclidian space $\mathbb{R}^d$ with $d \geq 1$. It must, however, be emphasized that the chirality of a figure is dependent on the dimension of the imbedding space. A figure which is chiral in the plane is achiral in space, since it can easily be mapped to its mirror image by a proper spacial movement. In general, a figure which is chiral in $\mathbb{R}^d$ loses its chirality in $\mathbb{R}^{d+1}$. Two chiral figures are said to be *enantiomer* (sometimes enantiomorphic) if one is a mirror image or the resultant of a proper movement of a mirror image of the other.

Asymmetric figures are always chiral, but the reverse is not true. A figure is chiral exactly if it contains only proper symmetries. When considering symmetries of chiral figures in the plane, rotations and translations can exist (Fig. 2) while glide reflections or (as a special case) reflections do not.

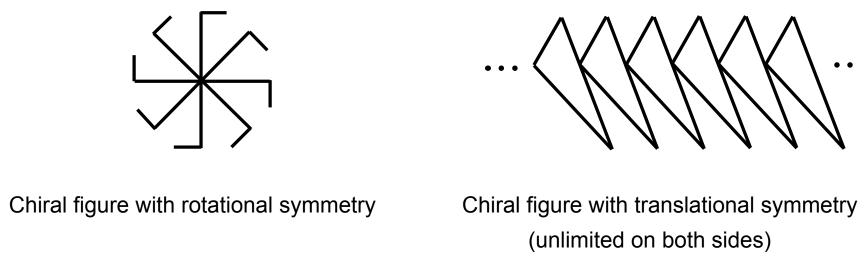


Fig. 2 Symmetric chiral figures of the plane

3 Reidemeister's criticism

After this short short presentation of the concept of chirality, we return to Kant's paradox. Which arguments does the mathematician Reidemeister use to counter the philosopher Kant? Reidemeister writes: *"The axioms of Euclidian geometry can be formulated as statements about distances between points and each theorem in geometry corresponds to a statement about distances between points. Leibniz was correct when he said that the geometrical properties of an object could be considered to be equal to the position of their parts."* In particular, the difference between enantiomer figures can thus be reduced to distances and with this, Reidemeister criticizes Kant's argument for the absolute space. It is not our purpose to comprehend the mathematical thoughts which led Reidemeister to this conclusion, but rather to interpret his result with the help of chirality.

Given three chiral figures, two of which are enantiomer; let them be denoted by A, A' (e.g. the two hands according to Kant) and B (e.g. one half of the body). Comparing the distances between A and B with the distances between A' and B, there will always be a difference. First, we want to specify this by using an example in the plane, which will also serve to illustrate the subsequent Theorem 3.1. Consider the chiral three-point figures $A = \{a_1, a_2, a_3\}$, $A' = \{a'_1, a'_2, a'_3\}$ and $B = \{b_1, b_2, b_3\}$ each of which form a scalene triangle (Fig. 3), then for at least one of the index pairs (i, j) with $i, j \in \{1, 2, 3\}$, the distances $\overline{a_i b_j}$ and $\overline{a'_i b_j}$ are different (see also [8]).

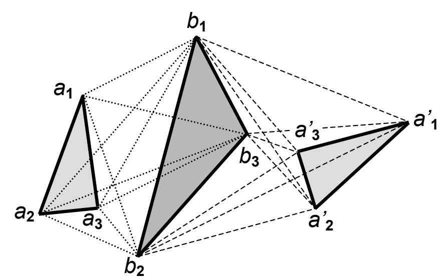


Fig. 3 Illustration of Theorem 3.1

Considering the general situation, it should be noted that the chiral figures A, A' and B need not be asymmetric. They can, as previously stated, have symmetries (besides the identity) which, however, must be proper.

Theorem 3.1. *Let A and A' be two enantiomer figures and B another chiral figure of $\mathbb{R}^d$. Furthermore, let ε be an isometry which maps A onto A' and σ a symmetry of B. Then there exist $a \in A$ and $b \in B$ with $\overline{ab} \neq \overline{\varepsilon(a)\sigma(b)}$.*

Proof (indirect). Assume that for all $a \in A$ and $b \in B$ there is $\overline{ab} = \overline{\varepsilon(a)\sigma(b)}$. Then there exists an isometry ϕ with $\phi(a) = \varepsilon(a)$ for all $a \in A$ and $\phi(b) = \sigma(b)$ for all $b \in B$. As, however, A, A' and B are chiral figures, they each have at least $d+1$ points in general position, and since an isometry of $\mathbb{R}^d$ is uniquely determined by $d+1$ points in general position and their images, it follows that $\phi = \varepsilon = \sigma$. This contradicts the assumption that σ is proper and ε improper . □

The quintessence of our interpretation of Reidemeister's result, as formulated in this Theorem 3.1, can be stated as follows: Enantiomer figures A and A' show a difference in distances if a metric relationship to another chiral figure B is considered. At the end of his work, Reidemeister adds that Kant's paradox would not have arisen had he furnished his absolute space with a Cartesian coordinate system. Thus, Reidemeister expresses that in mathematics, two enantiomer figures A and A' are differentiated by using a coordinate system as a chiral figure B. So much for the analysis of Kant's paradox. In the following section we will expound the practical applications of the result of this analysis.

4 Diachirality

Let us assume that our enantiomer figures A and A', as well as the chiral figure B, are (three-dimensional) objects in daily life or objects which occur in processes of nature. For the sake of simplicity, we will only consider rigid objects. Certain internal mobilities, such as is found in hands or molecules, will either be disregarded or replaced by a dynamic average. External movements, that is, movements of the objects as a whole, are permitted. Under these assumptions, Theorem 3.1 holds for any mutual positions of the objects A, A' and B and we call this phenomenon *diachirality*.

Due to the ever-present difference in distances caused by diachirality, certain interactions between A and B must differ from those between A' and B. Hence, there must be an observation that shows this difference. An important example in the history of chemistry is so-called optical activity: Two enantiomer, phase circular polarized, monochromatic light rays A and A' interact differently with a chiral molecule B, which generates a rotation of the oscillation plane of the resulting plane polarized light; one refers to the optical rotation of the molecule. In the case of equal wavelengths, the resulting angles of rotation of enantiomer molecules are reversed. It was through this observation in 1848 that the chemist Louis Pasteur first discovered chirality in molecules; he called his observation dissymmetry.

Diachirality is important particularly in pharmaceutical chemistry. Two enantiomer molecules A and A' contained in a medicament behave with respect to a chiral receptor B like two enantiomer keys with a chiral lock. If one of the two enantiomers A or A' fits B, then a physiological interaction occurs and the other enantiomer, because of diachirality, does not interact with the same receptor. In rare cases it can happen that the two enantiomers respond to two different receptors, which leads to different physiological reactions. Contergan (thalidomide), which was on the market between 1957 and 1961 as a mixture of enantiomers (Fig. 4) is a classic example. While one of the enantiomers (R-thalidomide) induces sleep as desired, the other (S-thalidomide) causes severe deformities in newborn babies (R and S refer to the sense of orientation dealt with in section 6). As a result of the Contergan scandal, 'chiral synthesis chemistry' has gained much in importance over the last few decades.

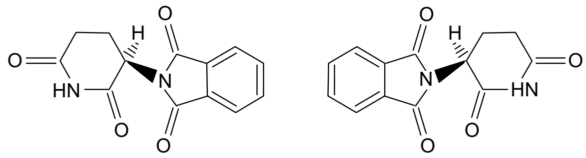


Fig. 4 Enantiomer molecules with different physiological effects

5 Chirality classes

To partition a set of chiral figures into two *chirality classes* means to form two subsets out of all the figures in such a way that enantiomer figures always belong to different subsets. If these figures are objects from daily life, the classes are usually identified by the words 'left' and 'right'; but it is irrelevant which term one chooses. Chirality classes are indispensable in communication, whether these be part of daily life or scientific in nature. A statement such as "I have lost my left glove" or "This flask contains R-thalidomide" refers to a partition of chiral objects into chirality classes. Forming chirality classes is always based on diachirality. For example, we consider one of two enantiomer shoes A and A' as belonging to foot B, since we unconsciously perceive distances between A and B which always differ from the corresponding distances between A' and B.

In chiral objects in nature we often find a common chiral structure, such as a spiral, which can be used to define chirality classes. Thus a snail's shell, a bean plant or even a double helix can be considered to belong to the same chirality class, if the involved spirals have the same spiral sense (note that this sense is the same from both axial sides). Be the way, Burgundy snails (Fig. 5) are usually clockwise; only one of thousands is anticlockwise, and there are said to be French gourmet restaurants which do not charge for the a meal if one of these is discovered on the plate.

turning clockwise turning anticlockwise

Fig. 5 Enantiomer Burgundy snails (turning anticlockwise rare)

6 Orientation

For many sets of chiral objects it is difficult to recognize a common structure which can be used to build chirality classes. How can 'potato-shaped' chiral figures or 'strangely-shaped' chiral molecules be associated, for instance, with a spiral or a hand? In principle, we need an enantiomer-maintaining procedure which ascribes complex chiral objects to a common chiral structure. In order for the procedure to be applicable in the same way to all chiral objects in the set under consideration, it has to be defined by uniquely determined rules, i.e., by an algorithm. We call such a procedure an *orientation* of the considered set of chiral objects. The terms (or symbols) which are used to identify the two chirality classes are said to be *sense of orientation*.

An important example of orientation in chemistry is a method devised by Cahn, Ingold and Prelog in the 1950's and is known today appropriately as the CIP-method. The symbols R (rectus) and S (sinister) are used to denote the sense of orientation. The CIP-method, which we cannot discuss here, has proved its value in practice, especially because it is based on established structural concepts. V. Prelog from the ETH Zurich received the Nobel Prize for Chemistry in 1975, also in recognition of his work in this field [8].

Starting in 1970, at the University of Zürich the authors and others developed a method which generates a unique name and the symmetry group of an internally mobile chemical structure which is based on a strict mathematical model. The underlying algorithm determines whether the structure is chiral or achiral and in the chiral case it provides an orientation [4]. The method does not depend on existing structural concepts and is suitable for computer implementation.[1]

In the second part of this work we shall use convex polytopes to explain the principle of this method which at the same time clarifies and makes concrete what has been said up to now. Convex polytopes are particularly suitable because, like chemical structures, they are based on finite sets of points.

7 Convex polytopes

The concept of a polytope is the d-dimensional generalization of the concept of a polygon for $d = 2$ and a polyhedron for $d = 3$ (Fig. 6). We shall restrict ourselves to convex polytopes, which allow a simpler presentation of the topics; the method can, however, be extended to non-convex polytopes. Convex polytopes are definable in several ways [5, 14]; we have chosen a definition which is most suitable for our purposes:

Definition 7.1. The convex hull P of a finite set of points in Euclidean space $\mathbb{R}^d$ ($d \geq 1$) with at least $d+1$ points in general positions is called a *convex d-dimensional*

[1] This project was supported since 1975 by the Swiss National Science Foundation.

polytope or, for short, a *polytope*. A point of a polytope P, which with respect to each line segment of P (connecting line of two points of P) is at most a boundary point, will be called a vertex of P; the vertexes form the *vertex set* X of P.

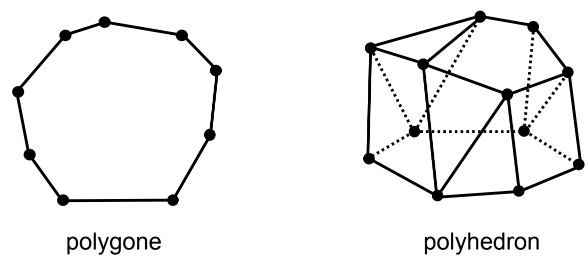


Fig. 6 Two-dimensional and three-dimensional polytope

Remarks

(1) A d-dimensional polytope will always be considered in $\mathbb{R}^d$ and not in a higher dimensional space, which is important regarding chirality.

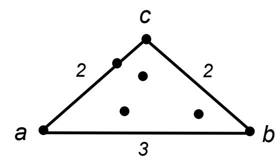
(2) As a convex hull, a polytope consists not only of its border, but also of its interior. Thus, a polygon is a surface and a polyhedron a solid, even though this is not expressed in the actual figures. For this work, however, it is irrelevant whether the interior of a polytope is included or not.

(3) We maintain without proof that a polytope is determined by the convex hull of its vertex set X, which forms a subset of at least $d+1$ vertexes in general position with respect to the original given finite set of points. Consider, for instance, the simple polygon, namely the isosceles triangle Tr (Fig. 7) which is defined as a convex hull of a set of 7 points, but is in fact determined by the vertex set $X=\{a,b,c\}$. By using methods from algorithmic geometry, X can be generated from the original set of points [1, 7]. In this work we always assume that a vertex set is already present.

(4) In the following we may speak of a *coordinate-dependent polytope* when the Cartesian coordinates of its vertexes are given and of a *coordinate-free polytope* if only the distances between the vertexes are known. The latter is merely determined up to isometry.

A coordinate-free polytope exists particularly if it is given in the form of a relational description or, simply, description. This expression shall be explained by using the example of our triangle Tr: We want to indicate the metric determined by the vertex set $X=\{a,b,c\}$ in a specific way. Each vertex connection is specified by the two corresponding vertex pairs which are symmetric to each other. Then the vertex pairs of isometric vertex connections are collected in so-called metric relations. The result is a 3-tuple: First we have the set X, followed by two metric relations which are ordered according to the distance squares 4 and 9 and named R_1 and R_2. We call this 3-tuple a description of Tr and write Desc(Tr) (for reasons of legibility the commas and parentheses of the vertex pairs are omitted).[2]

$$\mathrm{Desc}(Tr) = (X, R_1, R_2) = (\{a, b, c\}, \{ac, ca, bc, cb\}_4, \{ab, ba\}_9)$$



isosceles triangle Tr

Fig. 7 Polygon with the vertex set $X = \{a, b, c\}$

We can proceed in the same manner with any polytope. Whether we use the distance squares or the distances themselves to determine the order of the metric relation is irrelevant because of the monotonicity of the quadratic function defined on $\mathbb{R}^+$.

Definition 7.2. Let P be a polytope with the vertex set X and let t_1, t_2, ..., t_k be the distance squares occuring between the different vertexes with $t_i < t_j$ for $i < j$. Then the $(k+1)$-tuple $\mathrm{Desc}(P) = (X, R_1, R_2, ..., R_k)$ with the *metric relations* $R_i = \{pq \in X^2 \mid \overline{pq}^2 = t_i\}$ for $1 \leq i \leq k$ is called the *description* of P.

We now consider the automorphisms of the description of a polytope, which will play a central role in what is to come; we simply refer to the automorphisms of the polyope.

Definition 7.3. An automorphism of a polytope P with the description $\mathrm{Desc}(P) = (X, R_1, R_2, ..., R_k)$ is a bijection of the vertex set X onto itself which maps the vertex pairs of each metric relation R_i with $1 \leq i \leq k$ to a vertex pair of the same metric relation R_i. The automorphisms together with the composition as operation form a group, the *automorphism group* of P.

8 Minimizing concept

Before we apply the automorphism group of a polytope to problems of chirality and orientation, we will discuss a method which generates the automorphisms. The method is based on minimizing which was described in [12] for relational systems (a generalization of the descriptions of polytopes presented here). Minimizing is based on numberings:

Definition 8.1. Let n be the number of vertexes of the vertex set X of a polytope P. A bijection $\nu : X \to \{1, 2, ..., n\}$ is called a numbering of P.

[2]In contrast to the German version, the indices of the metric relations R_1 and R_2 are not the distance squares 4 and 9 but the successive numbers 1 and 2.

Minimizing involves three stages, in each of which all $n!$ numberings of a polytope P with n vertexes are taken into account. The three stages are formulated generally, but they are illustrated for the example of our triangle Tr in a Numbering table (Tab. 1).

	$\nu_i(a)$	$\nu_i(b)$	$\nu_i(c)$	number-descriptions $\nu_i(\mathrm{Desc}(Tr))$	canonizations $\langle\nu_i(\mathrm{Desc}(Tr))\rangle$
ν_1	1	2	3	$(\{1,2,3\},\{13,31,23,32\}_4,$ $\{12,21\}_9)$	$((1,2,3),(13,23,31,32)_4,$ $(12,21)_9)$
ν_2	1	3	2	$(\{1,3,2\},\{12,21,32,23\}_4,$ $\{13,31\}_9)$	$((1,2,3),(12,21,23,32)_4,$ $(13,31)_9)$
ν_3	2	1	3	$(\{2,1,3\},\{23,32,13,31\}_4,$ $\{21,12\}_9)$	$((1,2,3),(13,23,31,32)_4,$ $(12,21)_9)$
$\boldsymbol{\nu_4}$	**2**	**3**	**1**	$\boldsymbol{(\{2,3,1\},\{21,12,31,13\}_4,}$ $\boldsymbol{\{23,32\}_9)}$	$\boldsymbol{((1,2,3),(12,13,21,31)_4,}$ $\boldsymbol{(23,32)_9)=\mathrm{Min}(Tr)}$
ν_5	3	1	2	$(\{3,1,2\},\{32,23,12,21\}_4,$ $\{31,13\}_9)$	$((1,2,3),(12,21,23,32)_4,$ $(13,31)_9)$
$\boldsymbol{\nu_6}$	**3**	**2**	**1**	$\boldsymbol{(\{3,2,1\},\{31,13,21,12\}_4,}$ $\boldsymbol{\{32,23\}_9)}$	$\boldsymbol{((1,2,3),(12,13,21,31)_4,}$ $\boldsymbol{(23,32)_9)=\mathrm{Min}(Tr)}$

Tab. 1: Numbering table for Tr

Stage one: For each numbering of P, the letters in the description $\mathrm{Desc}(P)$ are replaced by the corresponding numbers. The results are the *number-descriptions* $\nu(\mathrm{Desc}(P))$.

Stage two: In each number-description $\nu(\mathrm{Desc}(P))$, the elements within the vertex set and within each metric relation are lexicographically ordered into tuples. The results are the *canonizations* $\langle\nu(\mathrm{Desc}(P))\rangle$.

Stage three: A lexicographically smallest canonization is chosen, the so-called *minimal canonization* $\mathrm{Min}(P)$. Note that $\mathrm{Min}(P)$ could be shortened; it would be sufficient to write only the lexicographically smaller of each symmetric pair.

The minimal canonization $\mathrm{Min}(P)$ can be considered as a uniquely determined name of the coordinate-free polytope determined by $\mathrm{Desc}(P)$. Names of this kind, which bear the total structural information, are useful in chemistry. We call numberings which result in the name $\mathrm{Min}(P)$ minimal numberings, or more formally:

Definition 8.2. A numbering of a polytope P is called a *minimal numbering* of P if $\langle\nu(\mathrm{Desc}(P))\rangle = \mathrm{Min}(P)$.

In the numbering table for the triangle Tr, the minimal canonization $\mathrm{Min}(Tr)$ appears twice, and thus there are two minimal numberings, namely ν_4 and ν_6. However, not only the minimal canonization but also the other canonizations occur twice, which has to do with the automorphisms of Tr. As can easily be seen, the following equivalence holds generally for two numberings ν and μ of a polytope P:

$$\begin{aligned} & \langle\nu(\mathrm{Desc}(P))\rangle \;=\; \langle\mu(\mathrm{Desc}(P))\rangle \\ \iff\quad & \alpha = \mu^{-1}\nu \text{ is an automorphism of } P. \end{aligned} \tag{8.1}$$

The set of all $n!$ numberings of a polytope P with n vertexes is therefore divided into classes which have as many numberings as automorphisms. Each of these *numbering-classes* can be used to determine the automorphisms by applying 8.1; here we work with the class of minimal numberings. For the triangle Tr, the minimal numberings ν_4 and ν_6 lead to the automorphisms $\alpha_1 = \nu_4^{-1}\nu_4$ and $\alpha_2 = \nu_4^{-1}\nu_6$ or written in cyclic notation:

$$\alpha_1 = (a)(b)(c), \;\; \alpha_2 = (c)(ab). \tag{8.2}$$

9 Minimizing algorithm

The minimizing concept just discussed involves the consideration of all $n!$ numberings of the n vertexes of a polytope. An algorithm based directly on this concept would be exponential and therefore impractical for larger values of n. We shall now present an algorithm which generates the minimal canonization and its associated minimal numberings without having to go through all n! numberings. How this minimizing algorithm works will be illustrated by using the example of a polyhedron with 5 vertexes, the triangular bipyramid Bp, whose vertexes lie on the surface of a cube with edge length 2 (Fig. 8). The description of Bp is as follows:

$$\begin{aligned}\mathrm{Desc}(Bp) = \big(&\{a,b,c,d,e\}, \{cd,dc\}_1, \{ae,ea,de,ed\}_4, \{bc,cb,ce,ec\}_5,\\ &\{ab,ba,ad,da,bd,db\}_8, \{ac,ca\}_9, \{be,eb\}_{12}\big).\end{aligned}$$

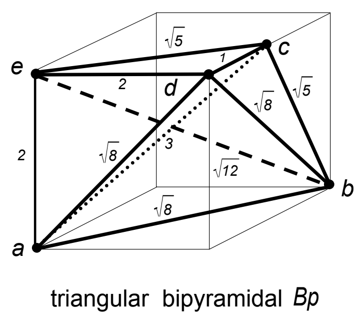


Fig. 8 Polyhedron with 5 vertexes in a cube with edge lengths 2

The minimizing algorithm is recursive and functions according to an Algorithm table (Tab. 2): In step 1, the two vertex pairs of the first metric relation of $\mathrm{Desc}(Bp)$ are minimized. After $r-1$ steps ($1 < r \leq 5$), we have *'description sequences'* with approriate lexicographically smallest *'minimal sequences'*. In the r-th step, these description sequences are extended by adding a further vertex pair: This extension occurs for each description sequence with every remaining vertex pair of the same metric relation or, if the latter is already completely worked off, with every vertex pair of the next metric relation of $\mathrm{Desc}(Bp)$. From the resulting description sequences, those which produce the lexicographically smallest minimal sequences will be used for the next step. By step 5, the algorithm can be stopped as only one lexicographically smallest minimal sequence remains and only number 5 is missing. We obtain a single minimal numbering - the associated automorphism $\alpha = \nu^{-1}\nu$ is the identity element - as well as the minimal canonization:

$$\nu : a \mapsto 4, b \mapsto 5, c \mapsto 2, d \mapsto 1, e \mapsto 3, \tag{9.1}$$

$$\begin{aligned}\mathrm{Min}(Bp) = \big(&(1,2,3,4,5),(12,21)_1,(13,31,34,43)_4,(23,25,32,52)_5,\\ &(14,15,41,45,51,54)_8,(24,42)_9,(35,53)_{12}\big).\end{aligned}$$

step r	description sequences	minimal sequences (lexicographically smallest bold faced)
1	$\boldsymbol{((cd,\ldots}$	$\mathbf{((12,\ldots}$
	$\boldsymbol{((dc,\ldots}$	$\mathbf{((12,\ldots}$
2	$\boldsymbol{((cd,dc)_1,(\ldots}$	$\mathbf{((12,21)_1,(\ldots}$
	$\boldsymbol{((dc,cd)_1,(\ldots}$	$\mathbf{((12,21)_1,(\ldots}$
3	$((cd,dc)_1,(ae$	$((12,21)_1,(34$
	$((cd,dc)_1,(ea$	$((12,21)_1,(34$
	$((cd,dc)_1,(de$	$((12,21)_1,(23$
	$((cd,dc)_1,(ed$	$((12,21)_1,(32$
	$((dc,cd)_1,(ae$	$((12,21)_1,(34$
	$((dc,cd)_1,(ea$	$((12,21)_1,(34$
	$\boldsymbol{((dc,cd)_1,(de,\ldots}$	$\mathbf{((12,21)_1,(13,\ldots}$
	$((dc,cd)_1,(ed$	$((12,21)_1,(31$
4	$((dc,cd)_1,(de,ae$	$((12,21)_1,(13,43$
	$((dc,cd)_1,(de,ea$	$((12,21)_1,(13,34$
	$\boldsymbol{((dc,cd)_1,(de,ed,\ldots}$	$\mathbf{((12,21)_1,(13,31,\ldots}$
5	$((dc,cd)_1,(de,ed,ae$	$((12,21)_1,(13,31,43$
	$\boldsymbol{((dc,cd)_1,(de,ed,ea,\ldots}$	$\mathbf{((12,21)_1,(13,31,34,\ldots}$
		$\nu : d \mapsto 1, c \mapsto 2, e \mapsto 3, a \mapsto 4$ and therefore $b \mapsto 5$

Tab. 2: Algorithm table for Bp

Even though the minimizing algorithm has not been stated here for the general case, the above example should suffice in describing its working principle. The algorithm does not play a central role in this work and a more thorough description for arbitrary relational systems can be found in [13][3]. It would be interesting to clarify the complexity of the minimizing algorithm where it applies to the descriptions of polytopes. In the example of our bipyramid, it is possible to stop the algorithm prematurely. In general, the maximum number of steps is equal to the total number of vertex pairs, i.e., $n(n-1)$ for a polytope with n vertexes whereby, in general, the number of description sequences varies with each step.

[3] In [13] 'canonization' is used in the sense of 'minimal canonization'.

10 Symmetry aspects

It is known that a symmetry of a d-dimensional polytope P is an isometry of the whole Euclidian space $\mathbb{R}^d$ which maps P onto itself. On the other hand, an automorphism of P only operates on the vertex set X. What is the relationship between the symmetries and the automorphisms?

Theorem 10.1. *For every symmetry of a polytope P, there exists exactly one automorphism of P with $\alpha = \sigma_X$ and conversely, whereby σ_X denotes the restriction of σ to the vertex set X.*

Proof. A given symmetry σ of P maps the vertex set X onto itself. Otherwise a vertex, which can be at most a boundary point of a line segment of P, would be mapped to the interior of a line segment of P, which leads to contradictions. Since σ maps every vertex connection to an isometric vertex connection, and therefore the image of every vertex pair will be a pair of the same metric relation, we have with $\alpha = \sigma_X$ exactly one automorphism of P. Conversely, given an automorphism α of P, then there exists at least one isometry σ with $\alpha = \sigma_X$. However, since a polytope has $d+1$ vertexes in general position, σ is uniquely determined (as already mentioned, a symmetry of $\mathbb{R}^d$ is uniquely determined by $d+1$ points in general position and their images). Moreover, the isometry σ is a symmetry of the whole polytope P, since this is the convex hull of the vertex set X. It may be noted that the biunique mapping between automorphisms and symmetries forms a group isomorphism. □

In the example of our isosceles triangle Tr, the unique mapping between the automorphisms (see 8.2) and the symmetries is evident: The assigned symmetry of α_1 is the identity and of α_2 an axis reflection (since c is fixed). In the case of the bipyramid Bp, the identity element is the only automorphism and Bp is therefore asymmetric. In general, however, an automorphism offers no clues as to the type of the assigned symmetry. The following example of two polygons serves as an illustration in this regard. We consider the isosceles trapezoid Tp and the parallelogram Pa (Fig. 9). In both cases, the minimal numberings and the automorphisms can be calculated by hand:

$$Tp: \quad \nu_1 : a \mapsto 4, b \mapsto 3, c \mapsto 1, d \mapsto 2, \quad \nu_2 : a \mapsto 3, b \mapsto 4, c \mapsto 2, d \mapsto 1,$$

$$\alpha_1 = (a)(b)(c)(d), \ \alpha_2 = (ab)(cd); \tag{10.1}$$

$$Pa: \quad \nu_1 : a \mapsto 4, b \mapsto 1, c \mapsto 2, d \mapsto 3, \quad \nu_2 : a \mapsto 2, b \mapsto 3, c \mapsto 4, d \mapsto 1, \tag{10.2}$$

$$\alpha_1 = (a)(b)(c)(d), \ \alpha_2 = (ac)(bd). \tag{10.3}$$

Although the automorphism groups of Tp and Pa determined by (10.1) and (10.3) are isomorphic permutation groups, their symmetries show a difference: With α_2 of Tp we have an axis reflection, however, with α_2 of Pa, a point reflection. In par-

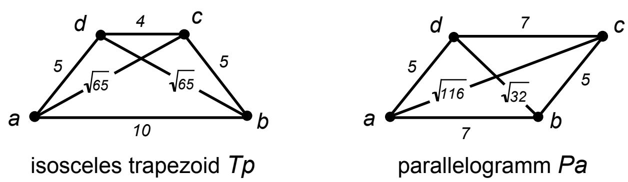


Fig. 9. Achiral and chiral polygon with isomorphic groups of automorphism.

ticular, by considering the structure of the two automorphism groups, it does not follow that Tp is achiral and Pa is chiral. In contrast, since the bipyramid Bp has only one automorphism, the identity element, we can conclude that Bp is chiral.

A procedure which examines whether a polytope is chiral shall be called a ***chirality test***. A chirality test consists primarily of an ***automorphism test***. It may be supplemented, if necessary, by a ***simplex test*** which will be described in section 12. With the automorphism test, one is trying to decide whether chirality exists purely based on the structure of the automorphism group. As we have just seen with the simple polygons Tp and Pa, there are cases where this is not possible. As an interesting question one may ask which necessary and sufficient conditions must be fulfilled such that the automorphism test leads to the goal. We do not know the complete answer, but mention a theorem which contains a simple sufficient condition:

Theorem 10.2. *A polytope is chiral if the order of its automorphism group is odd.*

Proof. We will show that the order of the automorphism group of an achiral polytope is even. The automorphism group and the symmetry group of a polytope have the same order (Theorem 10). The latter is, however, even for an achiral polytope, as the proper symmetries form a subgroup of index 2 and hence there are as many proper as improper symmetries. □

11 Oriented simplexes

In this section, we deal with oriented simplexes in order to prepare the above mentioned simplex test.

Definition 11.1. A d-dimensional polytope with $d+1$ vertexes is called a *d-dimensional simplex.* If, in addition, the vertexes are given in a particular order, we refer to an *oriented d-dimensional simplex.* In the following we simply speak of an *o-simplex*, denote it by S and write the vertexes as a $(d+1)$-tuple while adhering to the order, as for instance $S=(x_0, x_1, \dots, x_d)$.

Why do we speak of oriented resp. of o-simplexes? Due to the order of the vertexes, all coordinate-dependent o-simplexes of the same dimension can be oriented in the convential manner, i.e., with the help of determinant signs, even if they are achiral in the metric sense: If $S=(x_0, x_1, \dots, x_d)$ is an o-simplex, where x_0, x_1, $\cdots$, x_d are the coordinate representations of its vertexes, we consider the $d\times d$-matrix M_S, whose i-th row is the component vector $\overrightarrow{x_0x_i}$ $(1\le i\le d)$. If D denotes the determinant function, then let $\det(S):=\mathrm{D}(M_S)$. We have $\det(S)\neq 0$, since, by Definition 11.1, an o-simplex cannot be degenerate. And so we can define: Two d-dimensional o-simplexes S and T are equally oriented if $\det(S)$ and $\det(T)$ have the same sign, otherwise differently oriented.

Whether two o-simplexes S and T are equally or differently oriented can also be found in a single $d\times d$-matrix $M_{S,T}$ which takes into account the distances between the vertexes of S and T:

$$M_{S,T} = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1d} \\ m_{21} & m_{22} & \cdots & m_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ m_{d1} & m_{d2} & \cdots & m_{dd} \end{pmatrix} \tag{11.1}$$

$$\text{with } m_{ij} = 1/2\cdot\left(\overline{x_0y_j}^2 + \overline{x_iy_0}^2 - \overline{x_iy_j}^2 - \overline{x_0y_0}^2\right) \text{ for } i,j\in\{1,2,\dots,d\}.$$

By setting $\det(S,T) := \mathrm{D}(M_{S,T})$, we can state:

Theorem 11.1. *Two d-dimensional o-simplexes S and T are equally oriented exactly if* $\det(S,T)$ *is positive.*[4]

Proof. We show that the relationship

$$\det(S,T) = \det(S)\det(T) \tag{11.2}$$

is satisfied, which proves the theorem. For this we form the matrix product $M_SM_T^*$, where M_T^* is the transposed matrix of M_T. The (ij)-th element p_{ij} of this product is a scalar product which can be rearranged by using the vector identity $\overrightarrow{ab}\cdot\overrightarrow{ac} = 1/2\cdot\left(\overline{ab}^2 + \overline{ac}^2 - \overline{bc}^2\right)$ (cosine rule):

$$\begin{aligned} p_{ij} &= \overrightarrow{x_0x_i}\cdot\overrightarrow{y_0y_j} = \overrightarrow{x_0x_i}\cdot(\overrightarrow{x_0y_j} - \overrightarrow{x_0y_0}) = \overrightarrow{x_0x_i}\cdot\overrightarrow{x_0y_j} - \overrightarrow{x_0x_i}\cdot\overrightarrow{x_0y_0} \\ &= 1/2\cdot\left(\overline{x_0x_i}^2 + \overline{x_0y_j}^2 - \overline{x_iy_j}^2\right) - 1/2\cdot\left(\overline{x_0x_i}^2 + \overline{x_0y_0}^2 - \overline{x_iy_0}^2\right) \\ &= 1/2\cdot\left(\overline{x_0y_j}^2 + \overline{x_iy_0}^2 - \overline{x_iy_j}^2 - \overline{x_0y_0}^2\right). \end{aligned}$$

The last term shows that, according to (11.1), $p_{ij}=m_{ij}$ and thus $M_{S,T}=M_SM_T^*$. So we have:

$$\det(S,T) = \mathrm{D}(M_{S,T}) = \mathrm{D}(M_SM_T^*) = \mathrm{D}(M_S)\mathrm{D}(M_T) = \det(S)\det(T). \qquad \square$$

[4]The idea for this theorem comes from an unpublished work by Dimitrios Pazis (National Technical University of Athens), which he wrote as part of the project granted by the Swiss National Science Foundation mentioned in footnote 1.

It is also possible to determine the absolute value of $\det(S,T)$:

Corollary 11.1. If V_S and V_T are the volumes of two d-dimensional o-simplexes S and T, then

$$|\det(S,T)| = (d!)^2 V_S V_T. \tag{11.3}$$

Proof. (11.3) follows immediately, if one takes the absolute value on both sides of (11.2) and uses the well-known fact that $|\det(S)| = d!V_S$ and $|\det(T)| = d!V_T$. $\square$

We illustrate the results with two coordinate-free o-triangles (Fig. 10), namely $S = (x_0, x_1, x_2)$ and $T = (y_0, y_1, y_2)$. In order to determine the matrix $M_{S,T}$ according to (11.1), we need the following squared distances:

$$\begin{aligned}
\overline{x_0y_0}^2 &= 194, & \overline{x_0y_1}^2 &= 169, & \overline{x_0y_2}^2 &= 625,\\
\overline{x_1y_0}^2 &= 74, & \overline{x_1y_1}^2 &= 49, & \overline{x_1y_2}^2 &= 361,\\
\overline{x_2y_0}^2 &= 101, & \overline{x_2y_1}^2 &= 116, & \overline{x_2y_2}^2 &= 500.
\end{aligned}$$

We thus obtain $M_{S,T} = \begin{pmatrix} 0 & 72 \\ -20 & 16 \end{pmatrix}$ and hence $\det(S,T) = 1440$.

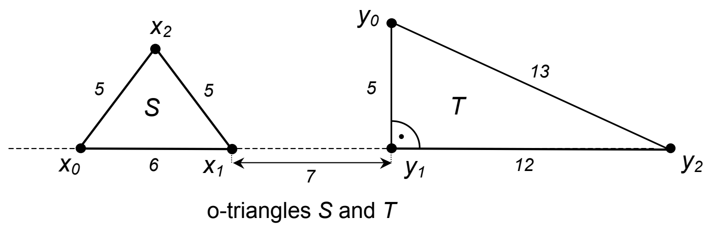


Fig. 10 Equally oriented two-dimensional o-simplexes

The determinant $\det(S,T)$ is positive and thus, according to Theorem 11.1, both o-triangles S and T are equally oriented. Their absolute value can be calculated by using Corollary 11.1: From $d=2$, $A_S=12$ and $A_T=30$, we obtain $|\det(S,T)| = 1440$. The determinant $\det(S,T)$ is either 1440 or -1440, depending on whether S and T are equally or differently oriented, respectively, and this will be the case for any mutual position of S and T. We add that the two signs of $\det(S,T)$ follow from Theorem 3.1 in an extended sense: The metrically achiral triangle S only achieves chirality through the different individualizations of its vertexes. Although this fact is important with respect to chemical models, we shall not go into more detail here.

12 Chirality of polytopes

What does the simplex test look like, in other words, how can we decide whether a polytope is chiral if the automorphism test is not sufficient? To answer this question, we work with an o-simplex $S = (x_0, x_1, \ldots, x_d)$ of a d-dimensional polytope P, i.e., the vertexes of S are now in particular vertexes of P. Apart from

S we also consider for an automorphism α of P the isometric o-simplex $\alpha(S) = (\alpha(x_0), \alpha(x_1), \ldots, \alpha(x_d))$ of P. The two o-simplexes S and $\alpha(S)$ are equally oriented exactly if the symmetry belonging to α is proper, independently of the o-simplex S of P under consideration. According to Theorem 10.2, the simplex test can be restricted to polytopes P whose order p of the automorphism group is even. And since all p symmetries for a chiral P and $p/2$ symmetries for an achiral P are proper, we finally obtain by using Theorem 11.1:

Simplex test. *Let P be a polytope with even order p of its automorphism group. To verify that P is chiral, one chooses an o-simplex S from P as well as $p/2$ automorphisms different from the identity element and tests whether the determinant* $\det(S, \alpha(S))$ *is always positive.*

Remarks

(1) For a coordinate-dependent P, it is appropriate to calculate $\det(S, \alpha(S))$ not by using the matrix $M_{S,\alpha(S)}$ according to (11.1), but rather with $\det(S)$ and $\det(\alpha(S))$. Indeed, by (11.2) we have $\det(S, \alpha(S)) = \det(S)\det(\alpha(S))$.

(2) It is often unnecessary to consider $p/2$ automorphisms different from the identity element. For example, in the case of a cyclic automorphism group, the restriction to a generating element is possible. The question of possible restrictions in general will not be discussed here.

We shall now perform the simplex test for the coordinate-free polygons Tp and Pa. In both cases we choose the o-triangle $S = (a, b, c)$ (see Fig. 9). With the single required automorphism α from (10.1) and (10.3), respectively, we obtain by calculation:

$$Tp : \det(S, \alpha_2(S)) = -1600, \text{ thus } Tp \textbf{ achiral},$$
$$Pa : \det(S, \alpha_2(S)) = 784, \text{ thus } Pa \textbf{ chiral}.$$

One-dimensional polytopes are line segments and thus always achiral. So the chirality concept is only of interest in the case of polygons, polyhedrons and polytopes of higher dimensions. We shall now examine a four-dimensional polytope Pt with regard to chirality. Pt is defined coordinate-dependent as the convex hull of the following 7 points:

$$a = (3, 2, 5, 3), \quad b = (3, 2, 1, 1), \quad c = (3, 6, 1, 3), \quad d = (4, 4, 5, 4),$$
$$e = (7, 3, 3, 4), \quad f = (5, 6, 2, 4), \quad g = (7, 2, 1, 3).$$

One can show: $S = (a, b, c, d, e)$ is not degenerate because $\det(S) \neq 0$, that is, the 5 points a, b, c, d and e are in general position and thus Pt is a 4-dimensional polytope. In addition, all 7 points lie on the surface of a 4-dimensional sphere with center $(3, 2, 1, 6)$ and radius 5; hence they are the vertexes of Pt. From the description of Pt, the minimizing algorithm[5] provides the minimal numberings. And since

[5]Here we used a programm developed by Ralf Gugisch (University of Bayreuth).

three minimal numberings and therefore three automorphisms are present, Pt is already chiral due to the automorphism test (Theorem 10.2); the simplex test is not needed. The minimal numberings are:

$$\begin{aligned}\nu_1 &: a \mapsto 2, b \mapsto 7, c \mapsto 4, d \mapsto 1, e \mapsto 5, f \mapsto 3, g \mapsto 6,\\ \nu_2 &: a \mapsto 4, b \mapsto 7, c \mapsto 6, d \mapsto 3, e \mapsto 1, f \mapsto 5, g \mapsto 2,\\ \nu_3 &: a \mapsto 6, b \mapsto 7, c \mapsto 2, d \mapsto 5, e \mapsto 3, f \mapsto 1, g \mapsto 4.\end{aligned} \tag{12.1}$$

13 Orientation of polytopes

An orientation of chiral polytopes of the same dimension shall now be defined on the basis of the minimizing concept. We start with a minimal numbering of a chiral d-dimensional polytope P. For each o-simplex $S = (x_0, x_1, \ldots, x_d)$ of P, we consider the corresponding numbered o-simplex $\nu(S) = (\nu(x_0), \nu(x_1), \ldots, \nu(x_d))$. We call the o-simplex S, which leads to the lexicographically smallest numbered o-simplex $\nu(S)$, a *reference simplex* of P and denote it by Ref_P. So, for each minimal numbering of P there exists a reference simplex Ref_P. Since each reference simplex is obtained from any other by an automorphism, all reference simplexes are isometric and, because of the chirality of P, equally oriented. This allows the following definition:

Definition 13.1. Two chiral d-dimensional polytopes P and Q are equally oriented if two reference simplexes Ref_P and Ref_Q are equally oriented, otherwise differently oriented.

Remarks

(1) An orientation is always somewhat arbitrary. In our procedure, two minimizings are undertaken, namely starting from the description of a polytope with a chosen order of the metric relations, a first in the choice of the numbering class and a second in the choice of the reference tuples with respect to this class.

(2) According to E. Ruch [10], there are special molecular classes which allow an orientation with 'physical relevance', inasmuch as with each continuous transformation of the physical parameters on the path from one chirality class to the other, an achiral state must be passed. In a similar way, continuity can be used to define an orientation with 'geometrical relevance' for special classes of polytopes.

For coordinate-dependent chiral d-dimensional polytopes, Definition 13.1 can obviously be implemented analytically by using a sense of orientation: If Ref_P is a reference simplex of such a polytope P, then P is *positively oriented* if $\det(Ref_P) > 0$ and *negatively oriented* if $\det(Ref_P) < 0$. For the perceptual spaces of dimensions $d = 2$ and $d = 3$, a well known illustrative sense of orientation is possible for the reference triangles and tetrahedrons, respectively, namely *right oriented* ('anticlockwise' or 'right hand rule') and *left oriented*. If one assumes a right-oriented coordinate system in the definition of the determinant, then positive and right-oriented as well as negative and left-oriented lead to the same chirality classes of polygons and polyhedrons. Note that even without using a sense of orientation, it can be decided whether two chiral d-dimensional polytopes P and Q are equally or differently oriented, provided one knows the mutual position of two reference simplexes Ref_P and Ref_Q. This is effected by using the sign of $\det(Ref_P, Ref_Q)$ according to Theorem 11.1.

Of the polytopes considered up to now, three are chiral, namely the parallelogram Pa ($d{=}2$), the bipyramid Bp ($d{=}3$) and the polytope Pt ($d{=}4$). In these three examples, we have the following sense of orientation:

Pa : Two minimal numberings ν_1 und ν_2 (10.2), we choose ν_1:
$Ref_{Pa} = (b, c, d)$, thus Pa **right** (see Fig. 9) resp. **positively oriented**;

Bp : Only one minimal numbering ν (9.1):
$Ref_{Bp} = (d, c, e, a)$, thus Bp **left** (see Fig. 8) resp. **negatively oriented**;

Pt : Three minimal numberings ν_1, ν_2 und ν_3 (12.1), we choose ν_2:
(e, g, d, a, f) und (e, g, d, a, c) are not reference simplexes (determinant 0),
$Ref_{Pt} = (e, g, d, a, b)$ with $\det(Ref_{Pt}) = 8$, thus Pt **positively oriented**.

14 Polygons and polyhedrons

The special (convex) polytopes, polygons and polyhedrons, permit a reduction of the number of vertex pairs of their descriptions such that the automorphism group generated with the help of the minimizing algorithm remains invariant. For a polygon or polyhedron with n vertexes, the quadratic number of vertex pairs $n(n–1)$ can theoretically be reduced to a linear number. In the following discussions, much remains merely indicated.

First we consider polygons with n vertexes. These are already uniquely determined up to isometry by the 'edge metric' (distances between any two successive vertexes on the boundary) and the first diagonal metric (distances between a vertex and the next but one on the boundary). The proof of this statement is inductive and essentially goes like this: One starts with a boundary triangle (triangle determined up to isometry consisting of two successive edges and a first diagonal) and with each induction step, by regarding the convexity, the next boundary triangle is added. In this way, the description, for $n \geq 5$, needs only $4n$ vertex pairs (per distance both pairs as usual). It is advisable to use separate metric relations for the edge and first diagonal metrics. In the special case of a regular polygon, the edge metric is sufficent, and the description has exactly one metric relation with $2n$ vertex pairs.

For polygons, the chirality test can be reduced to the automorphism test, since for the symmetry and thus the automorphism groups only the cyclic group C_m ($m \geq 1$) comes into question for chiral polygons and the Dieder group D_m ($m \geq 1$) for achiral polygons. The only exception is found in the group of order 2, where C_2 and D_1 are isomorphic and hence a simplex test may be necessary, as was shown in the example of the polygons Tp and Pa (see section 10).

As far as the polyhedrons with n vertexes are concerned, the reduction of the vertex pairs is based on Cauchy's Rigidity Theorem [3] from 1813. This theorem can be outlined as follows: Imagine a (convex) polyhedron whose boundary polygons are made of metal plates and whose edges have hinges, then the polyhedron is rigid. Or more precisely: A polyhedron is uniquely determined up to isometry by its 'boundary metric', i.e., what you see from the outside. (For the bipyramid Bp in Fig. 8, it would be superfluous to indicate the length of the vertex connection ac since it passes through the interior.) For the boundary metric, it is sufficient to regard, apart from the edge metric, the first diagonal metric of all the boundary polygons, here again with separate metric relations. With the help of Euler's Polyhedron Theorem, it can be proved that fewer than $10n$ vertex pairs need to be given for the description. In special cases, such as for regular or semi-regular polyhedrons, even a restriction to the edge metric is possible.

In contrast to polygons, the chirality test for polyhedrons may need a simplex test. When working 'coordinate-free', the simplex test generally requires knowledge of the distances between vertexes whose connecting segments pass through the interior of the polyhedron; the boundary metric is not sufficient.

How does one determine the vertex pairs which are to be used in the reduced description of polygons and polyhedrons? Normally, an additional algorithm is required to sort out these vertex pairs, and this may call into doubt the use of the reduction. It should be added that by Definition 13.1, another orientation of chiral polygons and polyhedrons is established if a reduced description is used instead of a complete one.

15 Closing remarks

There are many other interesting topics in connection with chirality. For example, the borderline between living and non-living nature has something to do with chirality. In living molecules, such as amino acids as the building blocks of proteins, only one of the two enantiomers is usually found. This phenomenon is known as homochirality and there have been various attempts at an explanation, and some of these lead to statistical problems [11]. The idea of a measure of chirality, that is, a measure for the deviation from achirality, is mathematically appealing. An interesting contribution was made by the group of the chemist K. Mislow (Dr.h.c. in 2002 of the University of Zurich) by using the geometric concept of the Hausdorff measure. An overview of the contributions to this topic is given in [2]. Another comprehensive work concerning chirality measure (unkown by publishing the German version of this paper) is given by Petitjean [15].

As far as we know, Kant was the first who carefully described the phenomenon of chirality with the help of enantiomer hands. Apart from its great practical value in modern chemistry, chirality is an appealing topic in the area which borders on philosophy, mathematics and natural science.

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[6] The meaning of 'Homochiralität' in [10] is slightly different from that of 'homochiral' in [11].
[7] See also on the internet: keyword 'homochirality'.